BIOGRAPHICAL SKETCH

NAME	POSITION TITLE
Whitfield, Troy W.	Postdoctoral Appointment

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
Boston University	Ph.D.	2002	Chemistry
University of Toronto	M.S.	1994	Chemistry
University of Toronto	B.S.	1992	Chemical Physics

Positions and Honors:

2005-present — Postdoctoral Appointee
Biosciences Division
Argonne National Laboratory
Argonne, IL

2002-2005 — Postdoctoral Researcher
I.B.M. Corporation
Yorktown Heights, NY Spring

Spring 2000 — Research Assistant
Moldyn Inc.
Cambridge, MA

1996-1999 — Teaching Assistant
Boston University
Boston, MA

1993-1994 — Teaching Assistant
University of Toronto
ON, Canada

Selected peer-reviewed publications

T.W. Whitfield and G.J. Martyna, “Ab-initio moledular dynamics studies of doping in single-wall carbon nanotubes,” (in preparation).

T.W.Whitfield andG.J.Martyna, “Modelingmany-bodypolarization and dispersion in molecular simulations: Solving the quantum Drude model in order-N,” (in preparation).

T.W. Whitfield and G.J. Martyna, “Internal energy estimation for path integration with harmonic actions,” J. Chem. Phys. (to be submitted).

T.W. Whitfield and G.J. Martyna, “A unified formalism for many-body polarization and dispersion: The quantum Drude model applied to fluid xenon,” Phys. Rev. Lett. (submitted).

T.W. Whitfield, J. Crain and G.J. Martyna “Structural properties of Nmethylacetamide via ab initio molecular dynamics, molecular dynamics and path integral molecular dynamics” J. Chem. Phys. (in press).

T.W. Whitfield, G.J Martyna, S. Allison, S.P. Bates, H. Vass and J. Crain “Structure and hydrogen bonding in neat N-methylacetamide: Classical molecular dynamics and Raman spectroscopy studies of a liquid of peptidic fragments,” J. Phys. Chem. B (in press).

T.W. Whitfield, G.J Martyna, S. Allison, S.P. Bates and J. Crain “Liquid NMA: A surprisingly realistic model for hydrogen bonding motifs in proteins,” Chem. Phys. Lett. 414 210(2005).

I. Andricioaei, T.W. Whitfield and J.E. Straub, “Generalized Monte Carlo methods for classical and quantum systems,” AIP Conf. Proc. 690 173 (2003).

T.W. Whitfield and J.E. Straub, “Gravitational smoothing as a global optimization strategy,” J. Comp. Chem. 23 1100(2002).

T.W. Whitfield, L. Bu and J.E. Straub, “Generalized parallel sampling,” Physica A 305, 157(2002).

T.W. Whitfield and J.E. Straub, “Enhanced sampling in numerical path integration: An approximation for the quantum statistical density matrix based on the non-extensive thermostatistics,” Phys. Rev. E 64, 066115 (2001).

T.W. Whitfield and J.E. Straub, “Uncertainty of path integral averages at low temperature,” J. Chem. Phys. 115, 6834(2001).